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Density functional theory study of GaSb(100) surface reconstruction JEFFERY HOUZE, Mississippi State University, SUNGHO KIM, Mississippi State University, SEONG-GON KIM, Mississippi State University — We use density functional theory to study the (100) surface of GaSb semiconductors. 2x2 reconstructions of the Ga and Sb terminating surfaces revealed the following patterns. The Ga terminating surface exhibits a pattern alternating between dimerization and buckling. The Sb terminating surface exhibits only dimerization with each pair alternating in height. Simulations of 2x3 reconstructions will be presented to indicate possibility of more complex patterns. Surface and reconstruction energies will be given in support of number of fixed layers used for simulating bulk, and number of free layers needed to adequately simulate the reconstructions. Charge density plots will also be presented to explain interaction between surface atoms.

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